PROGRESS IN NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

An International Review Journal

VOLUME 28

SUBJECT INDEX, AUTHOR INDEX
CONTENTS OF PREVIOUS VOLUMES

Executive Editors
J. W. EMSLEY and J. FEENEY

Consulting Editor
L. H. SUTCLIFFE

ELSEVIER

© 1996 Elsevier Science B.V. All rights reserved 0079-6565/96/$32.00 PER ARTICLE

No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior written permission of the publisher, Elsevier Science B.V., Copyright & Permissions Department, P.O. Box 521, 1000 AM Amsterdam, The Netherlands.
Upon acceptance of an article by the journal, the author(s) will be asked to transfer copyright of the article to the publisher. The transfer will ensure the widest possible dissemination of information.
Special regulations for readers in the U.S.A. — This journal has been registered with the Copyright Clearance Center, Inc. Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This consent is given on the condition that the copier pay through the Center the per-copy fee for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. The per-copy fee is stated in the code-line at the bottom of the first page of each article. The appropriate fee, together with a copy of the first page of the article, should be forwarded to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, U.S.A. If no code-line appears, broad consent to copy has not been given and permission to copy must be obtained directly from the author(s). The fee indicated on the first page of an article in this issue will apply retroactively to all articles published in the journal, regardless of the year of publication. This consent does not extend to other kinds of copying, such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works. Special written permission must be obtained from the publisher for such copying.
No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein.
Although all advertising material is expected to conform to ethical (medical) standards, inclusion in this publication does not consitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

The paper used in this publication meets the requirements of ANSI INISO 239.48—1992 (Permanence of paper),

Library of Congress Catalogue Card Number 66-17931

This issue is printed on acid-free paper.

PRINTED IN THE NETHERLANDS

ELSEVIER

PROGRESS IN NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Subject Index, Volume 28

A–60 41–42
Adiabatic regime 152–155
Ag(I) 311
^{27}Al, MAS 21
Alumina, metal fluorides 271
Aluminium fluorides 271, 273
Aluminophosphates 273
Aluminosilicates 272
Amino acids
  ^{1}H and ^{13}C chemical shifts 168–171
  ^{1}H NMR 211, 214
Angiography 118–120
Assignments 59

Backward linear prediction 258, 263
Barium aluminofluorophosphate glasses 271
Biological applications 4–5, 53–85
  cells and tissues 66–71
  in vivo 71–76
  nucleic acids 62–66
  proteins 55–62
Blood flow 76, 118
Blood oxygen level dependent (BOLD) 123
Bone 114
Bone implant materials 269
Bovine pancreatic trypsin inhibitor 61
Brain, ^{1}H NMR 73
Brain imaging 123
Bulk magnetic susceptibility shifts (BMS) 296

^{13}C chemical shift 163
  amino acids 168–171
  carbohydrates and polyols 174–179
  miscellanous metabolites 192–195
  nucleoside derivatives 184–186
  organic acids 172–173
  osmolytes 180–182
  solvents 196
  triacylglycerides 188–191
^{13}C MRS 75–76
^{13}C NMR 45
  cells and tissues 66
  metabolite profiles
    applications 214
    1D 191, 194–196
    2D 196–197
  shift and relaxation reagents 311
^{13}C–^{1}H HETCORR 196, 206–207
Calcium fluoride 268
Cancer 67, 211–212
Carbohydrates, ^{1}H and ^{13}C chemical shifts 174–179
Cardiac cine imaging 114
Cells and extracts 66–71, 210
Chemical shift 2, 162
  ^{13}C 163, 168–182, 184–186, 188–196
  ^{19}F 259, 264–268
  ^{1}H 162, 168–182, 184–186, 188–196, 209
  ^{139}La 304
  lanthanide induced 285–296
  ^{15}N 209
  ^{31}P 200–201
  solid surfaces 28
Chemical shift imaging (CSI) 72
Chemical shift reagents
  aqueous solution 312–314
  metal cation in biological systems 317–320
  organic solution 310–312
Chiral shift, lanthanide compounds 284, 314–316
Chlorofluorocarbons 278
^{35}Cl NMR 306
Clinical image contrast 106–112
Cloverite 273
COCONOSY 182, 198

Combined Rotation and Multiple Pulse Spectroscopy (CRAMPS) 23, 257, 261–262
^{19}F 268, 274, 276
Computer-assisted NMR 43–44
Computer of Average Transients (CAT) 3, 43–44
Conformational motion 16
Contact shifts, lanathanum 288–296
Continuous wave (CW) methods 19
Contrast agents, MRI 321
Gd(III) based 321
lanthanide complexes 322–335
COSY 46, 64, 178, 182–183, 187, 303
Coupling constants 164
^{1}H nuclei 163
triglycerides 188–191
nitrogenous compounds 209
Cross-polarization (CP) 258, 260
^{19}F NMR 274
Cross-polarization with magic angle spinning (CPMAS) 23, 25, 260, 341
Cryogenic imaging 33
^{63}Cu 18–19
Knight shift 225–228
NQR 221–225
nuclear relaxation in vortex cores 247
pair-breaking effect by magnetic impurity 248
spin-lattice relaxation rate 218–225
superconducting property 236–247
Cuprate superconductors 221–250
Curie spin contribution 299
Current shims 39–41
Cyclobutane 16

Dental enamel 268–269
Deoxyhemoglobin 122
DEPT 196, 205
DEPTH 258, 260
Depth-resolved surface coil spectroscopy (DRESS) 72, 126
Diamagnetic shifts 288
Diffusion, MRI 124
Dilute regime 150–152
DNA 62–66
Double resonance 23–24
Double rotation (DOR) 22
DQF-COSY 182–183, 199
d-wave 237–247
Dy(III) 289–291, 295, 311, 316–321, 335, 337
Dynamic angle spinning (DAS) 22
Dynamics in solids 14–16

Echo-planar imaging 98, 115–117
Electric field gradient 17, 223
Electromagnets 39
Electronic relaxation 333
Eu(III) 311
EXSY NMR 303–304, 323, 327

^{19}F chemical shifts 264–268
^{19}F MAS NMR 255–281
fluorinated polymers 278–280
inorganic fluorides 262–276
methodologies 257–262
small molecule 276–278
^{19}F NMR 26
in vivo 76
^{19}F–^{13}C dipolar coupling 276
^{19}F–^{31}P *J*-resolved spectroscopy 275
Fermion superconductors 237
Ferromagnetic materials 25
Field focusing NMR (FONAR) 91
Field gradient, Cu NQR 222
Field strength, MRI 109
FISP 114
FLASH 113–115
Flow-sensitizing gradients 119
Fluorescent lamp phosphors 270
Fluorides
inorganic 262–276
polymers 278–280
small molecules 276–278
Fluoroapatite 268–270
Flux stabilization 41
Force detection 33
Fourier transform (FT) 3–4, 20, 44, 92, 98–101
Fourier zeugmatography 92–98
Free induction decay (FID) 20, 44, 94, 112
Fullerines 31–32
Functional magnetic resonance imaging (fMRI) 74

Gallophosphates 273
Gallosilicates 272
Gd(III) 296, 299, 312, 321, 328, 330–335
Gd-DTPA 122–123
Glucose 75
Glycogen 75

Glycolate-lanthanide complexes 335
Gradient echo imaging 112–114, 120, 123
GRASS 114

^{1}H chemical shift 162
  amino acids 168–171
  carbohydrates and polycols 174–179
  lanthanide induced 295
  miscellanous metabolites 192–195
  nucleotide derivatives 184–186
  organic acids 172–173
  osmolytes 180–182
  solvents 196
  triacyglycerides 188–191
^{1}H coupling constants 163
  triacyglycerides 188–191
^{1}H NMR
  cells and tissues 66–68
  DNA 63
  in vivo 73
  metabolite profiles
    applications 210–214
    1D 166–167, 178, 208
    2D 178–179, 182–183, 208
  shift and relaxation reagents 311
^{1}H-observed — ^{13}C-edited MRS 75–76
^{1}H–^{31}P correlation spectroscopy 63
^{3}He 26
Heart 71, 114
Heme proteins 57
Heteronuclear Multiple Bond Correlation (HMBC) 48
Heteronuclear Multiple Quantum Correlation (HMQC) 47
Heteronuclear shift correlation spectroscopy (HETCORR) 46, 48, 190, 196, 206–207
Heteronuclear single quantum coherence (HSQC) 197, 201–203, 208
$HgBa_2Ca_2Cu_3O_8$ (Hg1223) 222, 225, 228, 230, 243–244, 247, 250
High resolution NMR 37–52
  1960s 42–45
  1970s 45–46
  1980s 46–48
  1990s 48–51
High temperature superconductors 30–31
HR-200 43

Image-slected *in vivo* spectroscopy (ISIS) 72–73
Imaging 5, 87–135
INEPT 196
Inner-sphere relaxation 297–301
Internal motion 155–156
In vivo spectroscopy 71, 125

J coupling 163–164

Klystron tube 38
Knight shift 18, 21, 31
  ^{63}Cu 225–229
  ^{17}K 228
  ^{17}O 228
  superconductors 239, 242

^{139}La NMR 304–307
  solid state 343
$La_{2-x}Sr_xCuO_4$ (LSCO) 222, 224, 228, 247–248
Lanthanide induced relaxation (LIR) 284–350
  biological systems 320
  contrast agents for MRI 321–335
  geometry calculations 307–310
  ^{139}La NMR 305
  reagents 310–320
  solid state NMR 340–343
  structure of reaction intermediates 335–340
  theory 296–303
Lanthanide induced shifts (LIS) 283–350
  biological systems 320
  contrast agents for MRI 321–335
  geometry calculations 307–310
  ^{139}La NMR 304–307
  reagents 310–321
  solid state NMR 340–343
  structure of reaction intermediates 335–340
  theory 285–296
  2D NMR 303–304
Lanthanides, electronic structure coordination behaviour 284
Laplace transformation 140
^{7}Li NMR 11, 16
  in vivo 76
Linewidth 18–19
Liouville equation 140–141
Liver metabolism 213
Ln (EDTA) 312–313, 340
Ln (DOTA) 313, 326–328

Ln (DTPA) 322–326
Ln (NOTA) 313–314
Ln(III) texaphyrins 328
Localized spectroscopy 125
Low-field regime 145–149
Lysozyme 57, 60

Magic angle spinning (MAS) 20–22
^{19}F 255–281
fluorinated polymers 278–280
inorganic fluorides 262–276
methodologies 257–262
small molecules 276–278
nanoprobe 50
solid surfaces 28
Magnetic impurity, pair-breaking 248
Magnetic materials 24
Magnetic resonance angiography (MRA) 118–120
Magnetic resonance imaging (MRI) 5, 87–130
blood flow 118
clinical image contrast 106–112
commercialization 103
functional (fMRI) 74
imaging speed 112–118
lanthanides as contrast agents 284–285, 304, 321
DOTA complexes 326–328
DTPA complexes 322
solution structures 322–328
structure-relaxivity 328–335
texaphyrin complexes 328
localized 125
neurogenic function 124
NMR microscopy 127
organ perfusion 121
scaling to human dimensions 102
Magnetic resonance spectroscopy (MRS), 72, 77, 125
^{1}H 73
^{13}C 75–76
^{31}P 74–75
Magnetic susceptibility agents 321
Magnetization transfer (MT) imaging 124
Magnets 3, 39
superconducting 19, 30, 42–43, 221–253, 271
Metabolite profiling
^{13}C chemical shifts 168–182, 184–186, 188–196
^{13}C NMR
applications 214
1D 191, 194–196
2D 196–197
^{1}H chemical shifts 168–182, 184–186, 188–196
^{1}H NMR
applications 210
1D 166, 208, 210–214
2D 178–179, 182–183, 186, 208, 214
^{15}N NMR 198–199
applications 215
1D 200–202
2D 202–203
^{31}P NMR
applications 214
1D 186
2D 187, 190
sample preparation 165
Metal cation shift reagents 317
Metal fluorides 271
Metals 18–19
Microprobes 49–50
MLEV 47
Molecular motion 12
Molecular tumbling 330
Montmorillonite clay, metal fluorides 272
Mössbauer lineshape 146
Motional-narrowing regime 149–150, 156
Multi-line scanning 114–118
Multiple pulse NMR 22–23
Multiple quantum NMR 29
Multiple sclerosis 107
Multipole operator basis 143, 146
Multi-slice imaging 106
Muscle disease 212

^{14}N chemical shift 2
^{14}N NMR, *in vivo* 76
^{15}N NMR 47
metabolite profiling 198–199
applications 215
1D 200–202
2D 202–203
^{15}N–^{1}H HSQC 212, 215
^{23}Na NMR 18–19
in vivo 76
Nanoprobes 50

Nd(III) 322–323
Negative temperature 16, 26
Niobium-zirconium wire 42
Nitrogenous compounds 209, 215
NMR
  biological applications 4–5, 53–85
  development of spectrometers 3–4
  early experiments 1–3
  high resolution 37–52
  imaging 5, 32, 87–135
  milestones in development 6–7
    solid state 11–36
NMR dispersion (NMRD) 301–303
NMR microscopy (NMRM) 127–128
NMR spectroscopic imaging 126
NOESY 64
Nuclear magnetic ordering 25–26
Nuclear Overhauser effect (NOE) 4, 24, 45, 61, 64–65, 164, 167, 304
Nuclear quadrupole resonance (NQR) 18, 147
  superconductors 221–225
Nucleic acids 62–66
Nucleoside phosphates, ^{13}P NMR 187

^{17}O Knight shift 228
^{17}O NMR 334
  shift and relaxation reagents 311
  solid state 341
^{17}O NQR 223
Oligonucleotides 64
One-dimensional ^{13}C NMR, metabolite profiling 191, 194–196
One-dimensional ^{1}H NMR, metabolite profiling 166
One-dimensional ^{15}N NMR, metabolite profiling 200–202
One-dimensional ^{31}P NMR, metabolite profiling 186–187
Organic acids, chemical shifts 172–173
$OTeF_5^-$ compounds 275
Outer sphere relaxation 302–303, 334
Outer volume suppressed image related *in vivo* spectroscopy (OSIRIS) 72
Overtone NMR 30

^{31}P MRS 74–75
^{31}P NMR 5
  cellular metabolism 66–68, 126
  DNA 63
  in vivo 71, 73
  metabolite profiles 186
    applications 214
    1D 186
    2D 187
^{31}P–^{1}H HETCORR 190
^{31}P–(^{1}H) relayed chemical shift correlation spectroscopy 191
Pair-breaking 239, 241, 244, 248
Peptides 60
Perfusion imaging 121
Perfusion techniques 69–71
Phase transitions 26
Phosphate metabolites
  ^{21}P chemical shifts 200–201
  ^{31}P NMR 214
Phosphomonoesters 74
Point resolved spectroscopy (PRESS) 72, 126
Polymers, ^{19}F MAS NMR 278
Polyols, chemical shifts 174–179
Polyurethane foams 278
Positron emission tomography (PET) 121, 126
Pr(III) 311
Proline 16
Proteins 5, 55–62
Proton decoupling, ^{19}F 277
Proton resonance frequency (MHz) 47–49
Pseudocontact shifts 291–296, 307
Pulse NMR 20
Pulsed field gradients 48
Pulsed Fourier transform 44

Quadrupole effect 16–18
Quadrupolar nuclei, spin dynamics 137–159
  adiabatic regime 152–155
  dilute regime 150–152
  internal motion 155–156
  locally anisotropic systems 142–145
  low-field regime 145–149
  motional-narrowing regime 149–150
  stochastic Liouville formalism 140–142

RARE 116–117
Relaxation 12, 15
  DNA 65
  internal motion 155
  ^{139}La 305
  lanthanide induced 284, 296–303

metals 18
superconductors 31–32, 228–235
tissue 106
vortex cores 247
Relaxation agents 122
aqueous solution 312–314
metal cations in biological system 317–320
organic solution 310–312
Reorientation 15
Resolvent superoperator 140, 143
Ribonuclease 55, 58–59
Ring-flipping 60
Rotating frame 19
Rotating frame zeugmatography 94
Rotational-echo double resonance (REDOR) 278–279
Ruderman–Kittel interaction 21

Scalar coupling 164, 167, 190
Self-diffusion 15, 19
^{29}Si MAS NMR 23–24
Signal intensity 164
Signal-to-noise ratio 3–4, 56–57, 60, 99, 102, 109–111, 128
Silica fluorides 274–275
Single photon emission tomography (SPECT) 121, 126
Skin effect 18
Sodalite 272
Solid state NMR 11–36, 340–343
Solid surfaces 27–28
Solomon–Bloembergen–Morgan (SBM) theory 329–330
Solvents 165
chemical shifts 196
SPARTAN 271
Spatial localization 91–92
Spatial resolution 32
Spectrometers, development 3–4
Spectroscopic imaging (SI) 125–126
Spin I 145–146, 149–154
Spin decoupling 41–42
Spin density operator 144
Spin diffusion 247
Spin dynamics, exchanging quadrupolar nuclei 137–159
adiabatic regime 152–155
dilute regime 150–152
internal motion 155–156
locally anisotropic systems 142–145
low-field regime 145–149
motional-narrowing regime 149–150, 156
stochastic Liouville formalism 140–142
zero-field evolution 156
Spin echo 2, 20, 44, 106, 108, 222
Spin glass 221
Spin Hamiltonian, quadrupolar nuclei 142
Spin-lattice relaxation 17–18
superconductors 32, 228–235
Spin Liouville space 140
Spin multiplicity 163
Spin-spin coupling 2, 39, 41
Spin temperature 16
Spin warp NMR imaging 94, 96–97, 112–114
Spiral scanning 117
SQUID 20
Sternheimer shielding factor 17
Stimulated echo acquisition mode (STEAM) 72, 126
Stochastic Liouville formalism 140–142
STRAFI 32–33
Structure in solids 12–14
Superconductors 19, 30–31, 42, 221–253
Knight shift 225–228
NQR frequency 222–225
nuclear relaxation in vortex cores 247
nuclear spin-lattice relaxation rate 228–235
pair-breaking by magnetic impurity 248–250
properties 236–247
substitutions 271
Surface coils 72, 125

Tb (III) 311
Temperature 15–16, 26
^{63}Cu Knight shifts 226, 229
superconductors 230–250
Texaphyrins, Ln(III) complexes 328
Three-dimensional imaging 102
Tin fluorides 275
$Tl_2Ba_2Ca_2Cu_3O_{10}$ (T12223) 222, 225–226, 230, 233–234, 243–245, 247, 250
$Tl_2Ba_2CuO_{6+y}$ (T12201) 222, 225–226, 230, 233, 236, 244, 250
Tm(III) 317–318

$(Tm(DOTP))^{5-}$ 319
TOCSY 46, 183, 186, 190, 196, 204, 207, 213, 303–304
Tooth enamel 268–269
Topical magnetic resonance 72
Transferred-echo double resonance (TEDOR) 278
Tumours 212
Two-dimensional HSQC 197, 202, 208
Two-dimensional INADEQUATE 48, 50–51
Two-dimensional NMR 45–47, 54, 90, 93
  ^{13}C, metabolite profiling 196–197
  ^{1}H, metabolite profiling 178–179, 182–183, 208
  lanthanide complexes 303–304
  ^{15}N, metabolite profiling 202–203
  ^{31}P, metabolite profiling 187, 190
  proteins 61
Two-dimensional ^{31}P–(^{1}H) relayed coherence transfer spectra 204
Two-dimensional spin warp imaging 99–100

Urea 13

Varian Associates 38
Vortex cores, nuclear relaxation 247

Water exchange rate 329–330, 334
Water of hydration, DNA 66
Water solvation number 290
Whole-body scanners 103–106, 109
Wigner-Eckart (WE) theorem 143, 145

^{129}Xe 28
XL-200 46

^{89}Y NMR 341
Yb(III) 311
$YBa_2Cu_3O_7$ 221–223, 227–230, 235–250

Zeolite
  ^{19}F MAS NMR 272
  $^{19}F/^{29}Si$ CPMAS 274
Zeugmatography 89–98
  scaling to human dimensions 102
Zero-field evolution 148, 156
Zero-field NMR 28–29
Zero-field splitting 303

ELSEVIER

PROGRESS IN NUCLEAR
MAGNETIC RESONANCE
SPECTROSCOPY

Author Index, Volume 28

Andrew, E.R., 11
Asayama, K., 221

Cohen, J.S., 53
Collier, S.W., 53

Emsley, J.W., 1

Fan, T.W.-M., 161
Feeney, J., 1

Halle, B., 137
Huskens, J., 283

Ishida, K., 221

Jaroszewski, J.W., 53

Kaplan, O., 53
Kitaoka, Y., 221

Miller, J.M., 255

Peters, J.A., 283

Raber, D.J., 283
Ruiz-Cabello, J., 53

Shoolery, J.N., 37
Szczesniak, E., 11

Wehrli, F.W., 87

Zheng, G.-Q., 221

ELSEVIER

PROGRESS IN NUCLEAR
MAGNETIC RESONANCE
SPECTROSCOPY

Contents of Previous Volumes

Volume 25

NMR and Fractal Properties of Polymeric Liquids and Gels
J. P. COHEN ADDAD

Sulfur-33 NMR
G. BARBARELLA

Photo-CIDNP of Biopolymers
P. J. HORE and R. W. BROADHURST

NMR Studies of Drug—DNA Interactions
M. S. SEARLE

NMR Studies of Dynamics in Nucleic Acids
A. N. LANE

Density Dependence of Rotational and Translational Molecular Dynamics in Liquids Studied by High Pressure NMR
E. W. LANG and H.-D. LÜDEMANN

Volume 26

NMR of Noble Gases Dissolved in Isotropic and Anisotropic Liquids
J. JOKISAARI

Characterization of Biomolecular Structure and Dynamics by NMR Cross Relaxation
R. BRÜSCHWEILER and D. A. CASE

Artifacts in Two-dimensional NMR
A. D. BAIN, I. W. BURTON and W. F. REYNOLDS

Copper–Zinc Superoxide Dismutase: A Paramagnetic Protein that Provides a Unique Frame for the NMR Investigation
I. BERTINI, C. LUCHINAT and M. PICCIOLI

Variable Angle Sample Spinning NMR in Liquid Crystals
J. COURTIEU, J. P. BAYLE and B. M. FUNG

Multinuclear and Multidimensional NMR Methodology for Studying Individual Water Molecules Bound to Peptides and Proteins in Solution: Principles and Applications
I. P. GEROTHANASSIS

^{17}O NMR Studies of Hemoproteins and Synthetic Model Compounds in the Solution and Solid States
I. P. GEROTHANASSIS

Fluorine NMR of Proteins
J. T. GERIG

Isotope Labeling in Solution Protein Assignment and Structural Analysis
D. M. LEMASTER

Magnetically-oriented Phospholipid Micelles as a Tool for the Study of Membrane-associated Molecules
C. R. Sanders II, B. J. Hare, K. P. Howard and J. H. Prestegard
NMR Studies of Complex Surfactant Systems
O. Söderman and P. Stilbs
NMR Studies of Translational Diffusion in Lyotropic Liquid Crystals and Lipid Membranes
G. Lindblom and G. Orädd
Recent Developments in Transferred NOE Methods
Feng Ni

Volume 27
Selenium-77 Nuclear Magnetic Resonance Spectroscopy
H. Duddeck
Chemical Shifts in Proteins Come of Age
L. Szilágyi
^{1}H NMR in the Structural and Conformational Analysis of Oligosaccharides and Glycoconjugates
E. F. Hounsell
^{1}H NMR Spectroscopy of Human Blood Plasma
M. Ala-Korpela
^{13}C Nuclear Magnetic Relaxation and Local Dynamics of Synthetic Polymers in Dilute Solution and in the Bulk State
P. Dais and A. Spyros
Hydration Water Molecules seen by NMR and by X-ray Crystallography
M. Billeter
^{2}H Zero Field NMR Spectroscopy
P. Jonsen